A sharp interface approach for compressible multiphase flow

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Abstract

The numerical simulation of compressible multiphase flow is a difficult task due to the close connection of thermodynamics and fluid dynamics. Our approach is based on a sharp interface treatment. The two phases are coupled by a ghost fluid method to avoid a mixing of the phases. To obtain information about the location of the interface a level-set equation is used. The bulk flows are approximated by a spectral element discontinuous Galerkin scheme for the Navier-Stokes equations that supports a general equation of state. To define values in the ghost cells, which establish the coupling of the two phases together with the propagation velocity of the phase front, we solve the multi-phase Riemann problem to determine the phase front velocity and to get the values at the phase interface from both sides, the liquid and the gas flow.

The focus of the talk will be the solution of the multi-phase Riemann problem itself. Two novel aspects of our current work are discussed in more detail. We present a first step in a comparison of the Riemann problem solution for the Euler equations with a microscopic solution based on molecular dynamics (MD) solution. The MD simulations are based on the Lennard-Jones model fluid with truncated and shifted potential, for which a highly accurate equation of state is available. This allows a clear connection of both simulations. However, the quite different time and space scales have to be bridged. We can show a perfect coincidence of these solutions for Riemann problems in the supercritical regime without occurring phase transitions. The other class of problems, addressed in the talk, describe expansion waves into vacuum, which allows simpler microscopic simulations. The MD simulation shows a clustering of molecules that is interpreted as a starting of droplet formation initiated by the strong pressure drop. We also show finite volume simulations for this case.

The other topic in the talk is the consideration of heat conduction that is important at phase transitions to balance the latent heat. Here, we propose a novel calculation of the numerical flux based on the generalized Riemann problem for advection diffusion problems. This is explained in detail for a scalar conservation law.